

Non-Gaussian normal diffusion induced by delocalization

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Non-Gaussian normal diffusion, i.e., the probability distribution function (PDF) is non-Gaussian but the mean squared displacement (MSD) depends on time linearly, has been observed in particle motions. Here we show by numerical simulations that this phenomenon may manifest in energy diffusion along a lattice at a non-zero, finite temperature. The models we study are one-dimensional disordered lattices with on-site potential. We find that the energy density fluctuations are spatially localized if the nonlinear interaction is suppressed, but may relax with a non-Gaussian PDF and a linear time-dependent MSD when the nonlinear interaction is turned on. Our analysis suggests that the mechanism lies in the delocalization properties of the localized modes.

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The non-Gaussian normal diffusion phenomenon was first evidenced experimentally in supercooled liquids [1, 2]. Later on it was also observed in the diffusive process of polystyrene beads on the surface of a lipid bilayer tube, of beads in an entangled solution of actin filaments [9], in soft matter systems [4–6], on polymer thin films [7], and in simulations of a two-dimensional system of discs [8]. It refers to the phenomenon that the probability distribution function (PDF) is non-Gaussian but the mean squared displacement (MSD) increases as time linearly. This phenomenon was believed to be common for particle diffusion in spatial and/or temporal heterogeneous medium, particularly in a variety of physicochemical and socioeconomic systems [9]. There are two conjectures about the mechanism. One assumes that a particle may experience different diffusion processes with different diffusion coefficients; though in each individual process it follows the normal Brownian motion, the composition of the individual Gaussian PDFs may result in an overall non-Gaussian profile [3, 9]. Another assumes that the particles have no memory of their diffusion directions, but may keep a positive correlation in the diffusion distance of each step [10]. Most of these studies have focused on the diffusion of particles, except Ref. [11], where the authors have studied a one-dimensional toy model consisting of particles and mobile walls arranged alternatively in a line. Kicking a particle in the middle of the system, the energy of the kick was found to spread in a non-Gaussian normal diffusion manner at certain parameters.

An important question arises: How general is this phenomenon? May it occur in the energy diffusion process in finite-temperature lattices? In this paper we show that non-Gaussian, normal energy diffusion may be common in disordered systems and occurs with delocalization. The Hamiltonian of the model we adopt is $H = \sum_k h_k$

with [12]

$$h_k = \frac{p_k^2}{2m_k} + \frac{(x_k - x_{k-1})^2}{2} + \frac{cx_k^2}{2} + \frac{\nu(x_k - x_{k-1})^4}{4}, \quad (1)$$

where p_k , m_k , and x_k are, respectively, the momentum, the mass, and the displacement from the equilibrium position of the k th particle. The lattice constant is set to unity, so that the number of the particles, denoted by N , also represents the length of the lattice. The masses of the particles distribute randomly and uniformly in the interval of (0.8, 1.2). The parameter ν controls the nonlinear interaction strength between particles; When ν vanishes, the model reduces to the disordered pinned harmonic (DPH) model, in which all the normal modes are localized if c is large enough. Recently, Dhar and Lebowitz have studied the heat conduction properties of this model by nonequilibrium simulations [12]. They found that the lattice shows a normal heat conduction behavior even if the nonlinear interaction is weak, implying that nonlinear interaction may induce a normal energy diffusive process. Conventionally, one may assume that this normal energy diffusive process is Gaussian, but we will show in the following it is non-Gaussian and is closely related to delocalization.

To start, we first determine the value of the parameter c that guarantees complete localization of normal modes in the DPH model. For this purpose, we employ the Thouless criterion which is widely adopted to identify localized and extended normal modes in condensed matter physics [13–15]. By simply changing the boundary condition from symmetric (with $x_1 = x_{N+1}$) to antisymmetric (with $x_1 = -x_{N+1}$) and calculating the frequency change, $\Delta\omega$, of a normal mode, the Thouless criterion states that it is localized if $\Delta\omega = 0$ or extended otherwise. In this way, we find that $c \geq 1$ can guarantee complete localization with the localization length being smaller than 3000. As such in the following we will focus

fig 1-wang

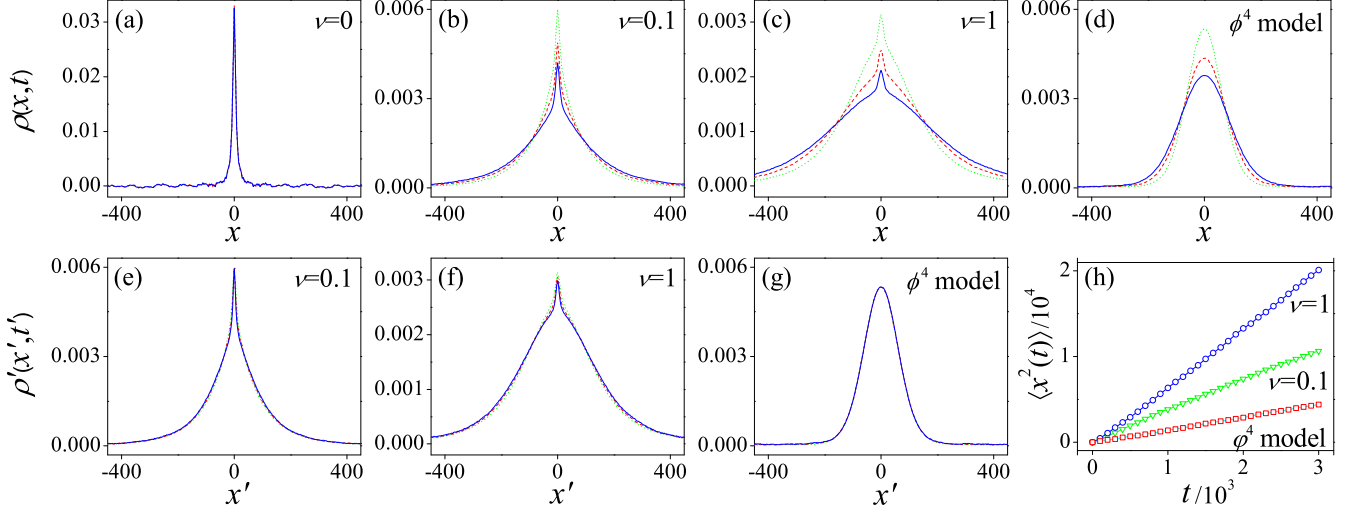


FIG. 1: (Color online) The spatiotemporal correlation functions of energy density fluctuations at time $t = 1000$ (green dotted line), 1500 (red dashed line), and 2000 (blue solid line) for the disordered lattice model with $\nu = 0$ (a), $\nu = 0.1$ (b), $\nu = 1$ (c), and for the homogeneous ϕ^4 model (d). Panels (e), (f) and (g) present the rescaled results given in (b), (c) and (d), respectively, with $t_0 = 1000$ (see text), and panel (h) is for the mean squared displacement of both models.

on the case of $c = 1$ and $N = 4096$. In addition, the energy density is set to be 1.5 as in Ref. [12].

To explore the diffusion behavior of energy in the equilibrium state at a non-zero, finite temperature, we investigate the spatiotemporal correlation function of energy density fluctuations. First of all, by numerically integrating the canonical motion equations, we evolve the system from a randomly assigned initial condition for a sufficient long time ($> 10^6$) to ensure that it has relaxed to the equilibrium state. We then divide the lattice into N_b bins of width b (in our simulations it has been set to $b = 4$) and calculate the spatiotemporal correlation function [16, 17]

$$\rho(x, t) = \frac{\langle \Delta e_j(t) \Delta e_i(0) \rangle}{\langle \Delta e_i(0) \Delta e_i(0) \rangle} + \frac{1}{N_b - 1}, \quad (2)$$

where $x \equiv (j - i)b$ is the distance between the i th and the j th bin and $\Delta e_j(t) = e_j(t) - e$ represents the energy fluctuation in the j th bin. $e_j(t) \equiv \sum h_k$, the summation involves all the particles in the j th bin at time t and e is the average energy of a bin. Because of the conservation of the total energy, there is a non-causal correlation term $-1/(N_b - 1)$ between different bins which should be excluded. This consideration leads to the last term in the equation [17]. The function $\rho(x, t)$ thus gives the causal relation between a local fluctuation and the effects it induces at another position at a later time, hence it is in essence equivalent to the probability density function that describes the diffusion process of the fluctuation. Taking advantage of this equivalence, $\rho(x, t)$ has been successfully applied to detecting the energy relaxation [16, 17] as well as the localization properties of a

fig 2-wang

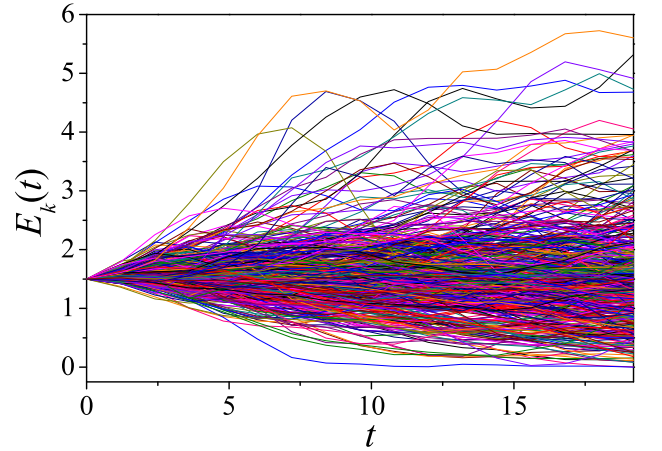


FIG. 2: (Color online) The energy of the normal modes of the disordered lattice with the nonlinear interaction parameter of $\nu = 0.1$. The diffusion behavior is a signal of delocalization.

system at a non-zero, finite temperature [18].

Figure 1(a) shows $\rho(x, t)$ for the DPH model (with $\nu = 0$) at different times. It can be seen that $\rho(x, t)$ does not decay, which is a clear signal of the energy localization. Meanwhile, it also indicates that $\rho(x, t)$ is an effective tool for identifying the localization feature in a non-zero temperature environment.

Introducing nonlinear interaction into our model may cause delocalization. Fig. 1(b) and (c) show $\rho(x, t)$ with $\nu = 0.1$ and 1, respectively. It can be seen that delocalization does occur and as a consequence, the height

fig 3-wang

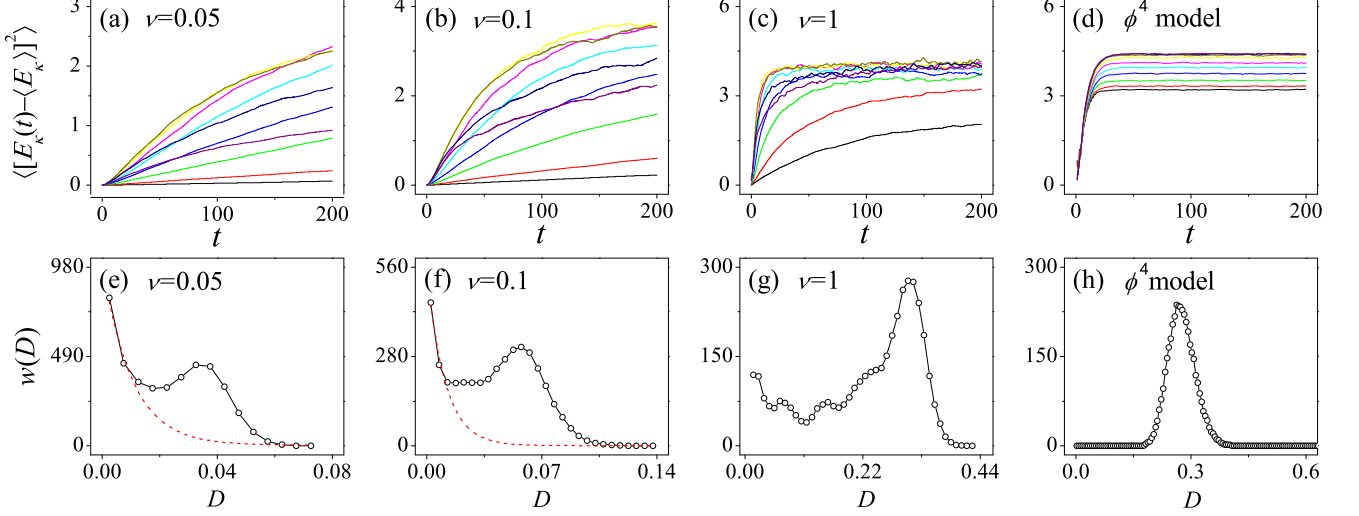


FIG. 3: (Color online) The energy diffusion among normal modes. Panel (a)-(c) show $\langle [E_k(t) - \langle E_k \rangle]^2 \rangle$ for the disordered lattice model with $\nu = 0.05, 0.1$ and 1 , respectively, and (d) for the homogeneous ϕ^4 model. Modes of $k = 409i$ with $i = 1, \dots, 10$ are taken as examples. Panel (e)-(h) show the distribution of the diffusion coefficient corresponding to (a)-(d). The dashed line in (e) and (f) indicates $\sim \exp(-aD)$, which is plotted for reference.

of $\rho(x, t)$ decreases as time (while the area under the $\rho(x, t)$ curve keeps unchanged since the energy is conserved). For the sake of comparison, Fig. 1(d) shows $\rho(x, t)$ of a homogeneous lattice, i.e., the ϕ^4 model, with $h_k = \frac{p_k^2}{2} + \frac{(x_k - x_{k-1})^2}{2} + \frac{x_k^2}{2} + \frac{x_k^4}{2}$. The ϕ^4 model has been shown to obey the Fourier heat conduction law [19].

We find that the function $\rho(x, t)$ of both systems follow the same scaling. By letting $t \rightarrow t' = t$, $x \rightarrow x' = x/\xi$, and $\rho \rightarrow \rho' = \xi\rho$ with $\xi = \sqrt{t/t_0}$ (t_0 is a reference time), the curves of $\rho'(x', t')$ at different times overlap perfectly [see Fig. 1(e)-(g)]. This scaling implies that $\langle x^2 \rangle = \int x^2 \rho(x, t) dx = (t/t_0) \langle x^2(t_0) \rangle$, i.e., the dependence of the MSD on time is linear. As Fig. 1(h) shows, the linear time-dependent behavior of the MSD can also be confirmed by calculating the MSD directly. Based on the results of the MSD, we know the energy diffusion is normal in both models. Meanwhile, in the homogeneous ϕ^4 model, $\rho(x, t)$ appears as a perfect Gaussian function, and therefore the energy diffusion in this model can be identified as the normal diffusion in the conventional sense.

However, $\rho(x, t)$ in the disordered model is obviously non-Gaussian. To explore the reason, we study the relaxation behavior of localized modes under nonlinear interactions. We first evolve the system up to a sufficient long time to have it relaxed to the equilibrium state, then we project the state of the system onto the normal modes of the DPH model, and record the time series of energy for each mode, $E_k(t)$, $k = 1, \dots, N$. With the vanishing nonlinear parameter, i.e., in the case of the DPH model, $E_k(t)$ is a time-independent constant governed by the ini-

tial condition as a consequence of localization. But with nonlinear interaction, energy exchange among different modes should take place and result in the diffusive motion of $E_k(t)$ in the energy space. As an example, in Fig. 2 we show $E_k(t)$ with $k = 8i$ for $i = 1, \dots, 500$ at $\nu = 0.1$. In this plot, the starting time for each $E_k(t)$ curve is set to be the time when $E_k(t)$ is sufficiently close to $\langle E_k \rangle$ with $|E_k(t) - \langle E_k \rangle| / \langle E_k \rangle < 0.01$ for the first time, where $\langle E_k \rangle$ represents the average energy of the k th mode at equilibrium. This treatment guarantees that the subsequent diffusion of $E_k(t)$ is around this reference energy. In the perfect equilibrium state with the energy equipartition, $\langle E_k \rangle$ should be the same for all the modes [20]. Fig. 2 indicates that delocalization takes place for all the modes. The diffusion is finally bounded since the total energy of the system is finite.

To further explore the diffusion rates of the normal modes we study the MSD $\langle [E_k(t) - \langle E_k \rangle]^2 \rangle$ as a function of time. Fig. 3 shows the MSD for $k = 409i$ with $i = 1, \dots, 10$ as examples. Fig. 3(a)-(c) are for $\nu = 0.05, 0.1$ and $\nu = 1$, respectively, and Fig. 3(d) shows the MSD for the homogeneous ϕ^4 model. The MSD curves are bounded finally as the total energy of the system is conserved. The fact that the MSD curves do not converge to the same value in the ϕ^4 model suggests that energy equipartition is not well fulfilled in this model. This phenomenon has been evidenced in this model when modes with smaller k have lower average energy at the equilibrium state [21]. In the case of the disordered lattice model, by tracking a sufficient long time we have found that $E_k(t)$ curves do mix with each other. In a shorter period of $t \leq 10$, $\langle [E_k(t) - \langle E_k \rangle]^2 \rangle$ depends on time al-

most linearly. We fit the slope in this period to measure the diffusion coefficient (denoted by D_k for the k th mode). In general, the values of D_k for different modes are different. Fig. 3(e)-(g) show the distribution of the diffusion coefficient [denoted by $w(D)$]; It can be seen that $w(D)$ approaches an exponentially decaying manner of $\sim A \exp(-aD)$ when $\nu \rightarrow 0$ in the two extreme ranges of D , meanwhile, there is a Gaussian-like peak in the range of moderate D . As ν increases, the peak becomes more and more dominant. In the case of the homogeneous ϕ^4 model, $w(D)$ shows only a Gaussian peak.

As mentioned previously, in order to explain the non-Gaussian normal diffusion phenomenon observed in particle motion, some authors have assumed that particles experience different diffusion processes with different diffusion coefficients and each individual process follows the normal Brownian motion [3, 9]. For our disordered lattice model a similar mechanism works. In fact, an initial energy fluctuation in the i th bin can be decomposed into normal modes, i.e., $\Delta e_i(0) \sim \sum_{k=1}^N \Delta e_i^{(k)}(0)$, where $e_i^{(k)}(0)$ denotes the component of the k th mode. Indeed, as shown in Fig. 3, these components proceed the normal diffusion with different diffusion coefficients, but it is in the energy space rather than along the lattice. So we assume that a component proceeds the normal diffusion in x space as well, i.e., $\rho^{(k)}(x, t) = (4\pi\bar{D}_k t)^{-\frac{1}{2}} \exp(-\frac{x^2}{4\bar{D}_k t})$, and its diffusion coefficient, \bar{D}_k , is proportional to D_k as $\bar{D}_k = \eta D_k$ with η being a constant. With this assumption, the PDF of $\Delta e_i(0)$ at time t is given by $\rho(x, t) = \frac{1}{N} \sum_{k=1}^N \rho^{(k)}(x, t)$, and $\langle x^2 \rangle = \frac{\eta}{N} (\sum_{k=1}^N D_k) t$. In other words, if only each component proceeds the normal diffusion, the MSD will be a linear function of time.

With this assumption we can also relate the profile of $\rho(x, t)$ to $w(D)$. Replacing the sum by integral in the thermodynamical limit of $N \rightarrow \infty$, we have

$$\rho(x, t) = \int_0^\infty w(D) \rho^{(k)}(x, t) dD. \quad (3)$$

In Fig. 4(a), $\rho(x, t)$ obtained with this formula for some assumed $w(D)$ has been plotted. For $w(D)$ being a Gaussian function, as in the case of the homogeneous ϕ^4 model, $\rho(x, t)$ would be a Gaussian function. For $w(D) \sim \exp(-aD)$, we have $\rho(x, t) \sim t^{-\frac{1}{2}} \exp(-\frac{|x|}{Ft})$ (F is a constant) and $\rho(x, t)$ has a Λ shape [9]. More importantly, if only $w(D)$ has a constant density close to $D = 0$, the PDF would show a non-Gaussian profile. Fig. 4(a) gives such an example with $w(D) = \text{constant}$ for $D < D_0$ and $w(D) = 0$ for $D \geq D_0$. We can see that $\rho(x, t)$ has a similar profile as the case of $w(D) \sim \exp(-aD)$. The reason is that components with close-to-zero diffusion coefficients relax slowly, and the smaller is D_k , the slower the relaxation is. On the contrary, if there are no components whose diffusion coefficients are close to zero, the center of $\rho(x, t)$ will show a Gaussian shape. In Fig. 4(a) $\rho(x, t)$ for $w(D) = 0$ for $D < D_0$ and $w(D) \sim \exp(-aD)$

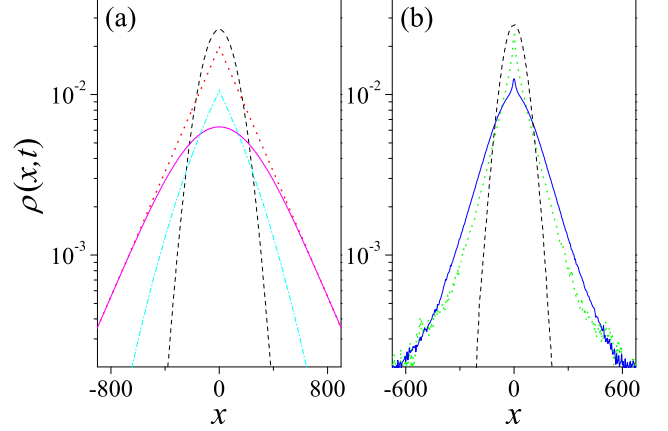


FIG. 4: (Color online) Panel (a) shows the profile of $\rho(x, t)$ based on Eq. (3) respectively for $w(D)$ being Gaussian (dashed line), for $w(D) \sim \exp(-aD)$ (dotted line), for $w(D) = 0$ if $D < D_0$ and $w(D) \sim \exp(-D/D_0)$ if $D \geq D_0$ (solid line), and for $w(D) = \text{constant}$ if $D < D_0$ and $w(D) = 0$ if $D \geq D_0$ (dash-dotted line). In panel (b), $\rho(x, t)$ in Fig. 1(b)-(d) with $t = 1500$ is plotted in the semi-log scale with the dotted, solid, and the dashed line, respectively.

for $D \geq D_0$ has been shown as an example; while the tails of $\rho(x, t)$ are exponential, the center is Gaussian.

Therefore, components with close-to-zero diffusion coefficients are crucial for the non-Gaussian profile, and delocalization may provide such components. In our disordered model, when the nonlinear interaction is suppressed, all modes are localized and the corresponding diffusion coefficients are zero. But when the nonlinear interaction is activated, delocalization happens but could be sufficiently slow if the nonlinear interaction is weak enough. As $w(D)$ is not zero near the origin even for $\nu = 1$, it explains why $\rho(x, t)$ shows a sharp peak around the origin [see also Fig. 4(b)]. In more detail, when nonlinear interaction is weak, the two ends of $w(D)$ fit the exponential decay [see Fig. 3(e)-(f)] and $\rho(x, t)$ has a Λ shape, suggesting that the close-to-zero diffusion components play the key role. When nonlinear interaction is stronger, the center peak of $w(D)$ becomes remarkable, and as a consequence, $\rho(x, t)$ deviates from the Λ shape.

In summary, relaxation of local energy fluctuations in the studied one-dimensional disordered system is featured by non-Gaussian normal diffusion. This finding suggests that non-Gaussian normal diffusion may be observed not only in certain specific complex systems but also in lattice systems, and not only in particle motion but also in energy relaxation. The mechanism is associated with delocalization of the localized normal modes. For weak enough nonlinear interaction, sufficient modes may relax sufficiently slow, which is a necessary condition for the non-Gaussian PDF.

Non-Gaussian normal diffusion observed in particle motion is believed to be a transient process in a proper time scale as diffusion is in principle a Markov process [9]. This conjecture may not apply to a lattice, because the number of modes is proportional to the lattice size and thus can be large enough, and small coefficients can be close to zero enough as well if nonlinear interaction is sufficiently weak. Therefore, the non-Gaussian PDF of energy can sustain long. Though a specific disordered lattice is studied here, the revealed mechanism may play a role in more general delocalization process.

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